

A semi-variance approach to visualising phylogenetic autocorrelation

Michael J. Noonan¹  | William F. Fagan² | Christen H. Fleming^{2,3} 

¹Department of Biology, The University of British Columbia Okanagan, Kelowna, BC, Canada

²Department of Biology, University of Maryland College Park, College Park, MD, USA

³Conservation Ecology Center, Smithsonian Conservation Biology Institute, Front Royal, VI, USA

Correspondence

Michael J. Noonan

Email: michael.noonan@ubc.ca; m_noona@live.concordia.ca

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Abstract

1. Comparing traits across species has been a hallmark of biological research for centuries. While interspecific comparisons can be highly informative, phylogenetic inertia can bias estimates if not properly accounted for in comparative analyses. In response, researchers typically treat phylogenetic inertia as a form of autocorrelation that can be detected, modelled and corrected for. Despite the range of methods available for quantifying the strength of phylogenetic autocorrelation, no tools exist for visualising these autocorrelation structures.
2. Here we derive variogram methods suitable for phylogenetic data, and show how they can be used to straightforwardly visualise phylogenetic autocorrelation. We then demonstrate their utility for three empirical examples: sexual size dimorphism (SSD) in the Musteloidea, maximum per capita rate of population growth, r , in the Carnivora, and brain size in the Artiodactyla.
3. When modelling musteloid SSD, the empirical variogram showed a tendency for the variance in SSD to stabilise over time, a characteristic feature of Ornstein–Uhlenbeck (OU) evolution. In agreement with this visual assessment, model selection identified the OU model as the best fit to the data. In contrast, the infinitely diffusive Brownian motion (BM) model did not capture the asymptotic behaviour of the variogram and was less supported than the OU model. Phylogenetic variograms proved equally useful in understanding why an OU model was selected when modelling r in the Carnivora, and why BM was the selected evolutionary model for brain size in the Artiodactyla.
4. Because the variograms of the various evolutionary processes each have different theoretical profiles, comparing fitted semi-variance functions against empirical semi-variograms can serve as a useful diagnostic tool, allowing researchers to understand why any given evolutionary model might be selected over another, which features are well captured by a model, and which are not. This allows for fitted models to be compared against the empirical variogram, facilitating model identification prior to subsequent analyses. We therefore recommend that any phylogenetic analysis include a nonparametric estimate of the autocorrelation structure of the data that can be visualised. The methods developed in this work are openly available in the new R package `ctpm`.

KEYWORDS

comparative methods, evolution, stochastic processes, variograms

1 | INTRODUCTION

Comparing traits across species has been a hallmark of biological research for centuries (Garland et al., 2005; Harvey & Pagel, 1991). Indeed, interspecific comparisons have yielded some of the most important biological advances, including the theory of evolution by natural selection (Darwin, 1859), allometric scaling rules (Bergman, 1848; Hirt et al., 2017; Jetz, 2004; Noonan et al., 2020; Rensch, 1950), the metabolic theory of ecology (Brown et al., 2004) and theories on the evolution of sociality (Lukas & Clutton-Brock, 2013; Noonan et al., 2015). While interspecific comparisons can be highly informative, as early as Darwin (1859) it was recognised that the characteristics of newly evolved species are based on modifications of traits inherited from ancestors. This inheritance will limit the differences in traits between closely related taxa, especially if only a short amount of time has passed, a phenomenon known as 'phylogenetic inertia' (Blomberg & Garland Jr, 2002). In his seminal paper, Felsenstein (1985) showed how phylogenetic inertia can be viewed as a form of statistical autocorrelation that could result in biased estimates and misleading significance if not properly accounted for in comparative analyses. Felsenstein (1985) effectively translated the concept of phylogenetic inertia into a statistical problem and provided a path forward for correcting for autocorrelation-induced biases in comparative analyses using statistical approaches.

The idea that phylogenetic inertia should leave a statistically identifiable autocorrelation structure in species trait data that could be modelled was transformative, and methods for modelling phylogenetic autocorrelation have evolved substantially over recent decades (e.g. Abouheif, 1999; Blomberg et al., 2020; Butler & King, 2004; Harmon et al., 2008; Martins & Hansen, 1997; Revell et al., 2008). Researchers now routinely model phylogenetic autocorrelation when making interspecific comparisons (Abouheif & Fairbairn, 1997; Johnson et al., 2017; Noonan et al., 2015), and/or quantify the strength of phylogenetic autocorrelation to infer evolutionary processes (Herrera, 2020; Kellermann et al., 2012; Morales, 2000). These approaches primarily rely on modelling evolution according to Gaussian stochastic processes, typically some form of Brownian motion (BM; Einstein, 1905), Ornstein–Uhlenbeck (OU) processes (Uhlenbeck & Ornstein, 1930), or, more recently, non-Gaussian stochastic processes (Blomberg et al., 2020). Models are fit via maximum likelihood estimation (Clavel et al., 2015; Harmon et al., 2008; Revell, 2012), and the best model is chosen via standard model selection procedures (Burnham & Anderson, 2002). While existing tools for working with phylogenetic data have yielded novel insight into evolutionary processes (e.g. Furness et al., 2021; Smaers et al., 2021), a challenge of the conventional workflow is that it offers no way to visualise the autocorrelation structure of the data, nor to assess whether any of the candidate models look like the data. This is a notable limitation as the ability to visualise autocorrelation

is crucial for understanding the underlying evolutionary process and determining what stochastic model the data best suggest. This stands in stark contrast to the numerous tools available for quantifying the strength of phylogenetic autocorrelation, such as Moran's I (Moran, 1950), Pagel's λ (Pagel, 1999), Abouheif's C_{mean} (Abouheif, 1999) and Blomberg's K (Blomberg et al., 2003) (reviewed in: Münkemüller et al., 2012). As a result of this limitation, researchers often rely on colouring the branch tips or lengths of phylogenetic trees based on trait values (e.g. Revell, 2013), or on plotting changes in diversity over time (Harvey et al., 1994). While these can serve as a useful visual tools, they provide only limited information on the underlying stochastic process by which a trait may be evolving.

Here we show how semi-variograms offer both a novel approach for visualising phylogenetic autocorrelation and a solution to the model diagnostic problem. Semi-variograms were originally developed to describe the degree of spatial dependence of random fields in geostatistics, as it was well known that geological samples taken close together in space would be more similar to one another than samples taken farther apart (Matheron, 1963). While originally developed to describe spatial autocorrelation, semi-variograms have also been extended to describe the temporal autocorrelation of stochastic processes (Fleming et al., 2014). Because the different stochastic processes used to model phylogenetic autocorrelation all have different theoretical variograms (Fleming et al., 2014), empirical semi-variograms can provide a useful diagnostic tool for checking a model's fit (Pérez-Barbería et al., 2004). Here, we extend semi-variograms to the needs of phylogenetic autocorrelation, develop confidence intervals on the estimated semi-variances, and implement the method into openly available software. We then demonstrate the utility of the method for three empirical examples: (a) the evolution of sexual size dimorphism (SSD) in the carnivoran superfamily Musteloidea (Noonan et al., 2016); (b) maximum per capita rate of population growth in the Carnivora (Fagan et al., 2013) and (c) brain size in the Artiodactyla (Haarmann, 1975; Oboussier, 1979).

2 | MATERIALS AND METHODS

2.1 | Semi-variograms for phylogenetic data

There are methods other than the variogram for visualising autocorrelation structures that can be applied to phylogenetic trait data. For instance, Gittleman and Kot (1990) and Diniz-Filho (2001) put forward methods for generating phylogenetic correlograms based on calculating Moran's I (Moran, 1950) at evenly spaced, user-defined distances classes and plotting this against the rank of the distance class. Although correlograms and variograms carry similar information, we focus here on semi-variograms

for three key reasons: (a) variograms have an unbiased estimator (Cressie, 1993), whereas this is not the case for correlograms; (b) variograms more readily relax the need for evenly spaced data (Fleming et al., 2014) and (c) variograms are better suited towards exploring the structure of autocorrelation in a dataset as opposed to correlograms that are typically used to identify the presence/absence of significant autocorrelation. Variograms are thus the only known unbiased, nonparametric autocorrelation estimator that can handle the highly irregular time intervals that typify phylogenetic tree data.

Let $x_i(t)$ denote the trait x of the ancestor of species i at time t in the past, which all share the same stochastic process distribution, but evolve independently after bifurcation. Under an assumption of stationarity, the semi-variance function at lag τ can be estimated via any weighted average of the form

$$\hat{\gamma}(\tau) = \sum_{i \neq j} w_{ij}(\tau) \underbrace{\frac{1}{2} |x_i(t) - x_j(t)|^2}_{\hat{\gamma}_{ij}(\tau)}, \quad \sum_{i \neq j} w_{ij}(\tau) = 1, \quad (1)$$

$x_i(\tau/2) \equiv x_i(\tau/2) \quad x_j(\tau/2) \equiv x_j(\tau/2)$

where the sum runs only over species that last shared a common ancestor at time $\tau/2$ in the past, and where the second constraint fixes the expectation value $E[\hat{\gamma}(\tau)] = \gamma(\tau)$. The above form of estimator is unbiased and asymptotically consistent, but its variance will be determined by our choice of weights $w_{ij}(t)$.

Optimal weights will minimise the variance

$$\text{VAR} [\hat{\gamma}(\tau)] = \sum_{i \neq j} \sum_{k \neq l} w_{ij}(\tau) w_{kl}(\tau) \text{COV} [\hat{\gamma}_{ij}(\tau), \hat{\gamma}_{kl}(\tau)], \quad (2)$$

under constraint (1). This, however, requires an estimate of the model. First, at a given lag τ , let us represent the above quadratic form in matrix notation as

$$\text{VAR} [\hat{\gamma}(\tau)] = \mathbf{w}^T \mathbf{\Sigma} \mathbf{w}, \quad (3)$$

where the indices of the block-vector $\mathbf{w}$ are ij and the indices of the block-matrix $\mathbf{\Sigma}$ are $ijkl$. When including constraint (1), the Lagrangian is

$$\mathcal{L}(\tau) = \mathbf{w}^T \mathbf{\Sigma} \mathbf{w} + \lambda (1 - \mathbf{1}^T \mathbf{w}), \quad (4)$$

where $\mathbf{1}$ is a vector of all 1s. The optimal weights are, via straightforward calculation, given by

$$\mathbf{w} = \frac{\mathbf{\Sigma}^{-1} \mathbf{1}}{(\mathbf{1}^T \mathbf{\Sigma}^{-1} \mathbf{1})}, \quad (5)$$

which requires inverting the covariance matrix $\mathbf{\Sigma}$. This, in turn, requires $\mathbf{\Sigma}$ to be correctly positive definite (PD). Therefore, we cannot reliably optimise our weights based on a nonparametric estimate of the variogram, because it will not be ensured to provide a PD covariance function. Instead, we can rely on parametric assumptions, as

all valid parametric models will always be PD. Moreover, we do not require all model parameters, as any overall constant (equivalent to the variance) will cancel out in (5). Given the stationary assumption, we only require the correlation matrix, $\mathbf{C}$.

$$\mathbf{w} = \frac{\mathbf{C}^{-1} \mathbf{1}}{(\mathbf{1}^T \mathbf{C}^{-1} \mathbf{1})}. \quad (6)$$

Here, our weights optimised to minimise variance can occasionally be negative, which can lead to slightly negative estimates when the true value is close to zero. This can be remedied by introducing the inequality constraints $w_{ij}(\tau) \geq 0$, which turns (5) into a quadratic programming (QP) problem that can be solved to obtain a non-negative estimate of less optimal variance (Turlach, 2019). In that case, the above relations still hold if the resultant QP weights are non-negative. In addition, the empirical variogram that we propose in Equation (1) is unbiased regardless of the true model (Cressie, 1993). When a parametric assumption about the form of the evolutionary process is also made, the variogram obtains the additional property of becoming optimal. We therefore focus on the independent and identically distributed (IID)-optimal and BM-optimal empirical variograms because they do not require any parameter estimates from the data. While this may seem like an extra restriction or assumption on the data, we note that the conventional empirical variogram and correlogram estimators used on time-series and spatial-field data are also only IID-optimal and could also be improved with optimal weighting (see e.g. Fleming et al., 2014).

2.1.1 | Independent and identically distributed

If the phylogenetic process is IID, then it is sufficient to consider the correlation matrix $\mathbf{C} \propto \mathbf{\Sigma}$, where the diagonal of $\mathbf{C}$ is 1 and the off-diagonal is 1/4 if species pair (i, j) and (k, l) share one species in common and 0 otherwise.

2.1.2 | Brownian motion

If the phylogenetic process is BM, then it is sufficient to consider the correlation matrix $\mathbf{C} \propto \mathbf{\Sigma}$, where the diagonal of $\mathbf{C}$ is 1 and the off-diagonal is the squared proportion of time-lag τ during which the backward-in-time-forward-in-time tip-branch-tip trajectories $\{x_i(0) \rightarrow x_{ij}(\tau/2) \rightarrow x_j(0)\}$ and $\{x_k(0) \rightarrow x_{kl}(\tau/2) \rightarrow x_l(0)\}$ correspond to the same species, where $x_i(\tau/2) = x_j(\tau/2) = x_{ij}(\tau/2)$ (Figure 1).

2.1.3 | Ornstein-Uhlenbeck

Optimal weights for an OU process can be derived, but there will be dependence on the unknown time-scale parameter, which is why we do not consider such cases here.

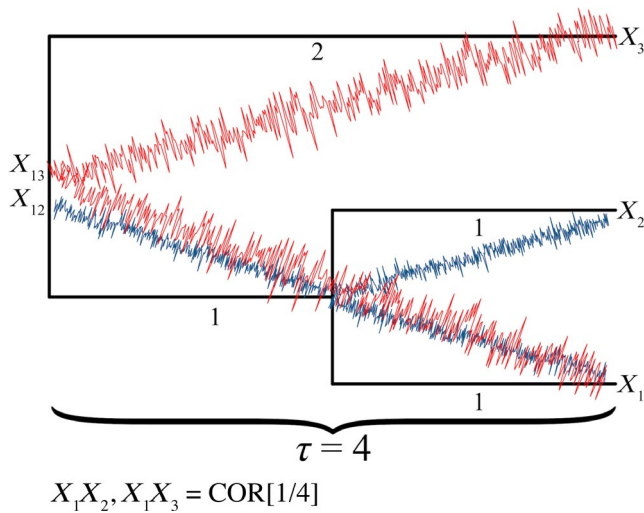


FIGURE 1 Schematic diagram depicting the calculation of the Brownian motion weights for a trait X between the species pairs (1, 2) and (1, 3)

2.1.4 | Confidence intervals

Using the same weights as before, and assuming the correlation structure to be correct, the variance of the variogram is given by

$$\text{VAR}[\hat{\gamma}(\tau)] = 2(\mathbf{w}^T \mathbf{C} \mathbf{w}) \hat{\gamma}(\tau)^2. \quad (7)$$

Variances are strictly positive and range between 0 and ∞ , so as an improvement over normal confidence intervals, which can include negative values, we summarise the uncertainty in $\hat{\gamma}(\tau)$ with χ^2 statistics.

2.1.5 | Time-lag gridding

The time-lags for phylogenetic variograms are calculated based on the topologies and branch lengths of the supplied phylogenetic trees (phylograms or chronograms), and the structure of a particular tree will dictate what pairwise time-lags are possible. These trees represent snapshots of the evolutionary processes, and will almost always result in irregular time series. Although irregularity in the data is acceptable, coarsening the variogram according to time-lag bin widths can make variograms more straightforward to interpret. Here we identify the lag bins using Gaussian mixture model (McLachlan & Basford, 1988) and k -means (MacQueen et al., 1967) clustering implemented in the R package `clusterR` (ver 1.2.4, Mouselimis, 2021), with the number of clusters, n , given as $n = \sqrt{n_{\text{lags}}} + 1$, and initial estimates of the centroids given by the regular grid points running along the range of lags. This number of bins was selected as in the limit of a perfectly regular time series, the number of bins would reduce back to the conventional grid.

The methods developed in this work are openly accessible in the new R package `ctpm`, version 1.0.1 available on CRAN.

2.2 | Semi-variance functions of evolutionary models

We next express IID, BM and OU models in terms of their semi-variance functions. We selected these three processes as they are the models most frequently used in practice (e.g. Fagan et al., 2013; Furness et al., 2021; Pérez-Barbería et al., 2004; Smaers et al., 2021). We also provide a biological interpretation of the parameters of these three semi-variance functions. A diagram of how these semi-variance functions relate to different tree configurations and patterns of traits assumed under each model is shown in Figure 2. Furthermore, in Appendix S1 we provide the full details of a simulation study aimed at exploring the relationship between the IID, BM and OU evolutionary models, their semi-variance functions, and the resulting empirical semi-variograms. For these simulations, the number of tips in the simulated trees and the number of replicates were held consistent across all simulations, and only the underlying evolutionary model was changed. We then visually assessed the empirical variogram against the evolutionary process that generated the trait values, and quantified the coverage of the 95% confidence intervals.

2.2.1 | IID: No phylogenetic inertia

Under an IID model of evolution, the values of traits observed in lineage i at one point in time $x_i(t)$ are independent of traits at any other time $x_i(t')$, with $t \neq t'$ and evolve according to a white noise process. In other words, there is no phylogenetic autocorrelation present under this evolutionary model and the semi-variance is therefore not dependent on the time-lag τ , but is simply given by the steady-state variance

$$\gamma(\tau) = \sigma^2. \quad (8)$$

The IID model is unlikely in most data, however, it does serve as a null model against which comparisons can be made. For instance, if only a small number of distantly related species are being compared, there may be no statistically detectable phylogenetic autocorrelation in the trait data.

2.2.2 | BM: Infinitely diffusive evolutionary process

Brownian motion describes a random walk with a fixed mean and a conditional variance that is proportional to the amount of time that has passed, diverging to infinity in the limit of infinite time. Its semi-variance function is given by

$$\gamma(\tau) = D |\tau|, \quad (9)$$

where D is the diffusion rate of the process and is proportional to the variance that can be expected over any given time-lag. Under a BM model of evolution, traits are free to evolve without constraint. The

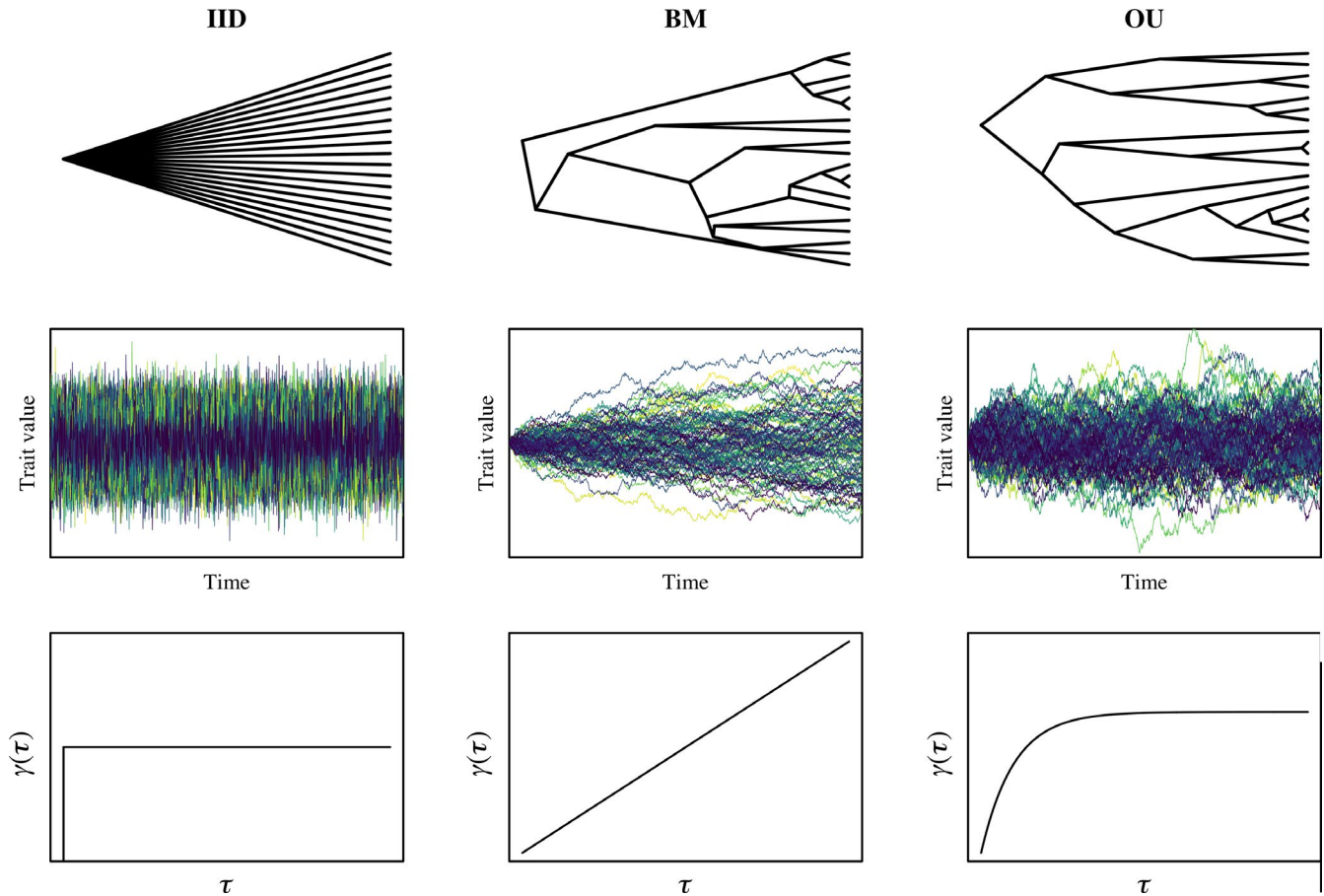


FIGURE 2 Examples of independent and identically distributed (IID), Brownian motion (BM) and Ornstein-Uhlenbeck (OU) phylogenetic models and their semi-variograms. The first row depicts the form of the phylogenetic tree assumed under each processes, the second the underlying stochastic processes, and the third the theoretical semi-variance functions. In particular, note how the BM and OU phylogenetic trees are difficult to differentiate, whereas the semi-variance functions can be easily distinguished

semi-variance function, therefore, increases without bound over time. BM is likely most relevant when studying highly plastic traits, or comparing traits across taxa that have only recently diverged.

2.2.3 | OU: Diffusive evolutionary process with mean reversion

The OU process generalises BM by specifying an upper limit on the process, σ^2 , centred around a mean. Within the bounds of σ^2 , the trait undergoes a random search for an optimal value but with a tendency to stay near the mean. The semi-variance function for the OU model of evolution is

$$\gamma(\tau) = \sigma^2 (1 - e^{-|\tau|/\tau_x}), \quad (10)$$

where τ_x is a trait's mean-reversion time-scale ($\tau = 1/\alpha$ in Martins, 1994), and σ^2 is the variance of the process ($\sigma^2 = \sigma^2/2\alpha$ in Martins, 1994). The OU process is equivalent to the BM process in the limit of no central tendency, $\tau_x \rightarrow \infty$, and infinite divergence, $\sigma^2 \rightarrow \infty$, with fixed diffusion rate $D = \sigma^2/\tau_x$. The OU process

represents a variation of Brownian diffusion when $\tau \ll \tau_x$, and, due to the central tendency, asymptotes to a constant variance when $\tau \gg \tau_x$. In other words, BM and OU can be indistinguishable over short time-scales because a trait has not yet diverged sufficiently far from the mean and it is only over longer time-lags that it is possible to tell the difference between BM and OU processes. In the limit where $\tau \rightarrow 0$, $D = \sigma^2/\tau_x \rightarrow \infty$ and the OU process converges to an IID model of evolution.

2.3 | Empirical case studies

2.3.1 | Musteloid sexual size dimorphism

We first demonstrate the utility of semi-variograms for modelling the evolution of SSD in the carnivoran superfamily Musteloidea. Musteloids are an ecologically diverse group of carnivores that exhibit substantial variability in SSD, ranging from parity, to males being more than twice the size of females (Noonan et al., 2016). Here we use a dataset describing SSD in 48 species of extant musteloids gathered by Noonan et al. (2015). We paired these data

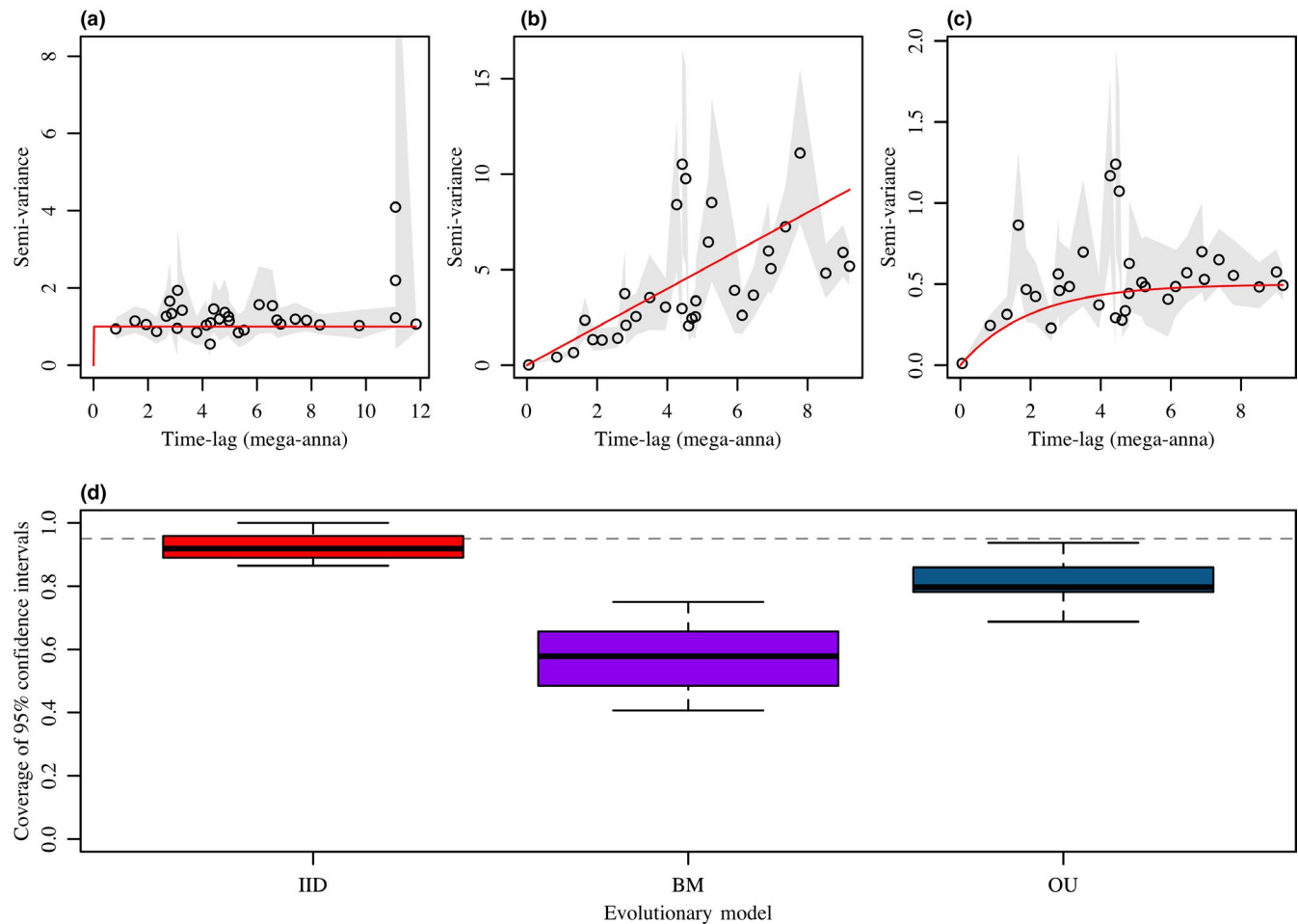


FIGURE 3 Empirical semi-variograms estimated from trait data that were simulated via (a) and independent and identically distributed (IID) process with no phylogenetic inertia; (b) and infinitely diffusive Brownian motion (BM) process; and (c) a diffusive Ornstein–Uhlenbeck (OU) process with mean reversion. In (d) boxplots of the coverage across 20 replicates are shown

with a time-scaled phylogenetic tree of the musteloids compiled by (Law et al., 2017, Figure 4a). For these data we estimated the empirical semi-variogram using the BM weights described above, and fit IID, BM and OU processes to the data using the methods implemented in the R package *slouch* (ver 2.1.4; Kopperud et al., 2020).

2.3.2 | Carnivora maximum per capita rate of population growth (r)

We next demonstrate the utility of phylogenetic semi-variograms for modelling maximum per capita rate of population growth, r , in the Carnivora, a central measure of population biology. We use a dataset describing r in 63 species of extant carnivores gathered by Fagan et al. (2013). We paired these data with a phylogram of the Carnivora compiled by (Agnarsson et al., 2010, Figure 5a), with branch lengths computed by Fagan et al. (2013). The r values were log-scaled prior to analysis and the empirical semi-variogram and model fitting process were carried out as described above.

2.3.3 | Artiodactyla brain size

Finally, we apply phylogenetic semi-variograms when modelling the evolution of brain size in the Artiodactyla, which represents the even-toed ungulates. Here we used morphological data on log-scaled mean brain size (g) described in Haarmann (1975) and Oboussier (1979), and openly available in the R package *slouch*. We paired these data with a phylogenetic tree of the Artiodactyla compiled by (Toljagić et al., 2018, Figure 6a), also available in *slouch*. Again, the empirical semi-variogram and model fitting process were carried out as described above.

The R script required to reproduce these analyses is presented in Appendix S2.

3 | RESULTS

3.1 | Simulation study

From our simulation study, we found that there was generally good correspondence between the true evolutionary models and

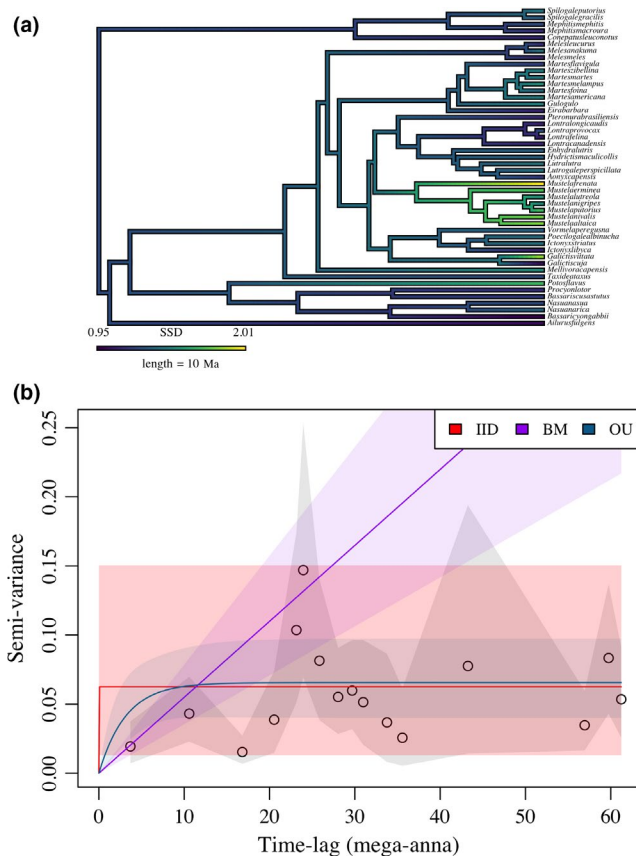


FIGURE 4 Phylogenetic tree (a) and semi-variogram (b) on musteloid sexual size dimorphism (SSD). The colours in the scale bar in (a) depict SSD values while the length of the bar is scaled to 10 Ma

the empirical variograms (Figure 3a–c; for full details see Appendix S1). Importantly all key features of the true semi-variance functions from which the trait data were simulated could be easily seen, highlighting the utility of this approach as a visual diagnostic tool. We found that the coverage of the confidence intervals in the IID and OU cases was near nominal, however, the coverage for the BM model was lower than expected (Figure 3d). Although the coverage was lower than 95% on average, the point estimates showed good correspondence with the true model (Figure 3b). This suggests that the lower than expected coverage was not due to biased point estimates, but rather confidence intervals that were unduly narrow.

3.2 | Musteloid SSD

When modelling musteloid SSD, AICc based model selection identified the OU process as the best fit to the data, although with marginal support for an IID model (Table 1). There was substantially less support for the BM model. While the AICc values provided support for SSD evolving according to an OU process, they provide no information on why this model was selected over the BM or IID processes, nor on why an IID model had substantially more support

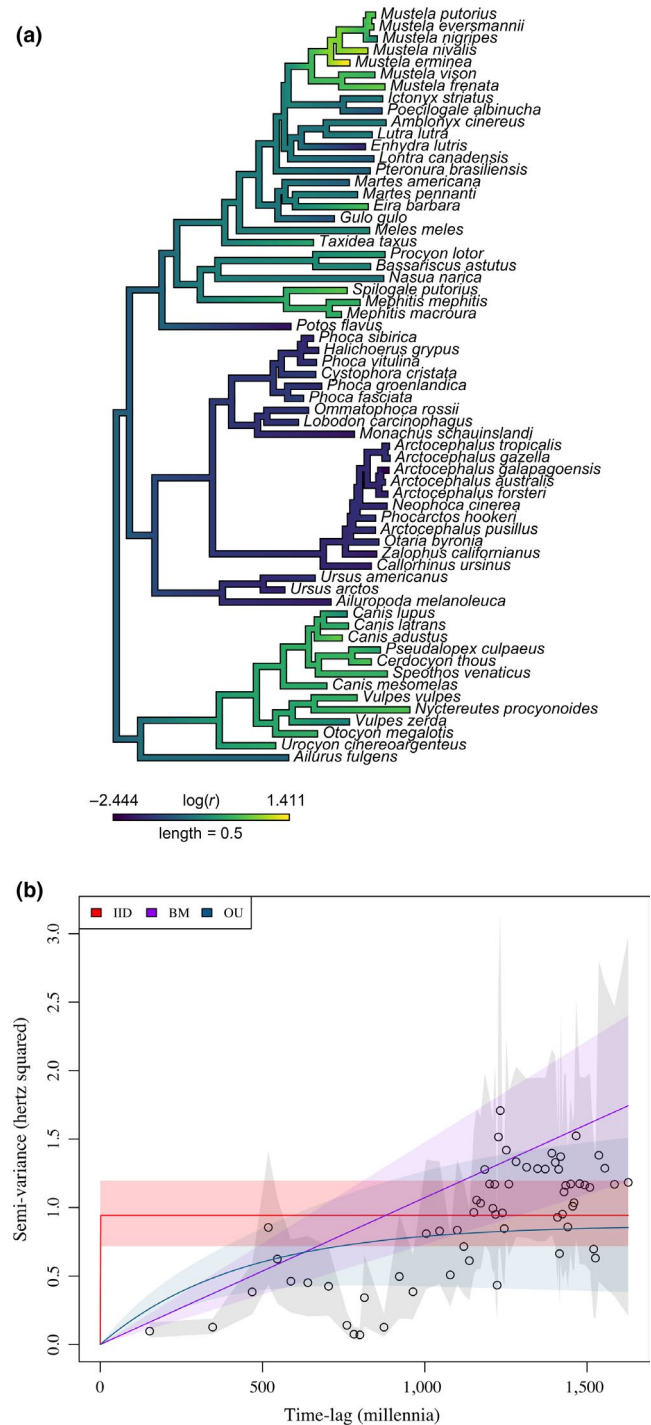


FIGURE 5 Phylogenetic tree (a) and semi-variogram (b) on maximum per capita rate of population growth, r , in the Carnivora. Note here the application of the method to a phylogram as opposed to the chronograms in Figures 4 and 6. The colours in the scale bar in (a) depict r , while the length of the bar is scaled to 0.5 arbitrary units of time on the phylogenetic tree

than BM. Comparing the fitted models against the empirical semi-variogram demonstrates the reason for the preference of the OU model over the BM or IID processes (Figure 4b). The empirical semi-variogram for the variance in SSD shows clear asymptotic behaviour. The infinitely diffusive BM model was the least supported based on

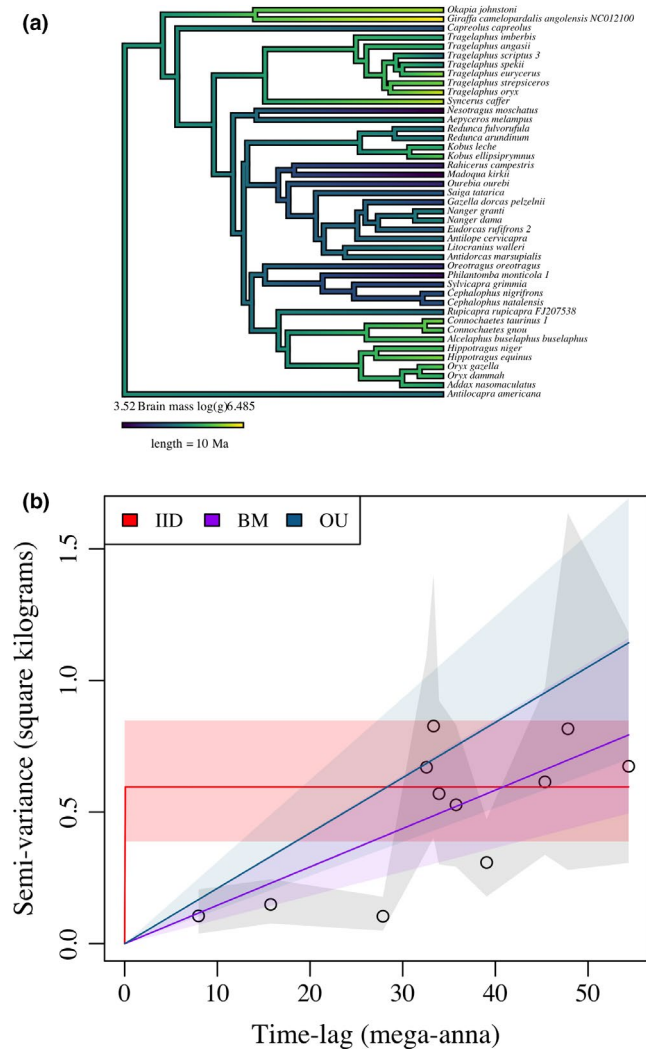


FIGURE 6 Phylogenetic trees (a) and semi-variogram (b) for brain size in the Artiodactyla. The colours in the scale bar in (a) depict brain sizes while the length of the bar is scaled to 10 Ma

TABLE 1 Small-sample-size corrected Akaike information criterion (AICc) differences for models fit to musteloid sexual size dimorphism. In the first three columns the diffusion rate (D , in mega-anna⁻¹), phylogenetic autocorrelation time-scale (τ_{SSD} , in mega-anna), and stationary variance (σ^2), are shown. The evidence ratios for each model were calculated as $1/e^{-1/2\Delta AICc}$

Model	D	τ_{SSD}	σ^2	$\Delta AICc$	Ev. ratio
OU	0.03	3.16	0.066	0	1
IID	∞	0	0.062	2.5	3.5
BM	0.01	∞	∞	15	1,808

Abbreviations: BM, Brownian motion; IID, independent and identically distributed; OU, Ornstein–Uhlenbeck.

AICc values, and the semi-variogram clearly shows this mismatch. The IID model, in contrast, captures the asymptotic behaviour of the empirical variogram, but misses the phylogenetic autocorrelation over shorter time-scales. Only the OU model captures both features of the semi-variogram.

TABLE 2 Small-sample-size corrected Akaike information criterion (AICc) differences for models fit to the log-scaled maximum per capita rate of population growth, r , in the Carnivora. In the first three columns the diffusion rate (D , in proportional units of time⁻¹), phylogenetic autocorrelation time-scale (τ_r , in proportional units of time) and stationary variance (σ^2), are shown. The evidence ratios for each model were calculated as $1/e^{-1/2\Delta AICc}$

Model	D	τ_r	σ^2	$\Delta AICc$	Ev. ratio
OU	2.84	0.43	0.87	0	1
BM	2.14	∞	∞	2	2.7
IID	∞	0	0.94	56.6	1.9×10^{12}

Abbreviations: BM, Brownian motion; IID, independent and identically distributed; OU, Ornstein–Uhlenbeck.

TABLE 3 Small-sample-size corrected Akaike information criterion (AICc) differences for models fit to artiodactyla brain size data. In the first three columns the diffusion rate (D , in mega-anna⁻¹), phylogenetic autocorrelation time-scale (τ_r , in mega-anna) and stationary variance (σ^2), are shown. The evidence ratios for each model were calculated as $1/e^{-1/2\Delta AICc}$

Model	D	τ_r	σ^2	$\Delta AICc$	Ev. ratio
BM	0.03	∞	∞	0	0
OU	0.03	4.3×10^5	9.1×10^3	2.4	3.3
IID	∞	0	0.77	31.3	6.3×10^6

Abbreviations: BM, Brownian motion; IID, independent and identically distributed; OU, Ornstein–Uhlenbeck.

3.3 | Carnivora r

We found that the evolution of the intrinsic rate of increase, r , in the Carnivora was best described by an OU process (Table 2), with the empirical semi-variogram showing clear asymptotic behaviour (Figure 5b). In other words, the best fit model suggests that population growth rates are not expected to evolve without bound, but instead fluctuate around a mean. Here, although the IID model was able to capture the asymptotic behaviour of the variogram, it missed the phylogenetic inertia over shorter evolutionary time-scales. As a result it received $\sim 1.9 \times 10^{12}$ times less support than the OU model and $\sim 7.5 \times 10^{11}$ less support than BM.

3.4 | Artiodactyla brain size

For brain size in the Artiodactyla, AICc based model selection identified the BM process as the best fit to the data, although with marginal support for an OU model, and substantially less support for the IID model (Table 3). Again, while the AICc values provided support for brain size evolving according to a BM process, they provide no information on why this model was selected over the OU or IID processes. Comparing the fitted models against the empirical semi-variogram demonstrates the reason for the preference of the BM model over the OU or IID processes (Figure 6b). In contrast to the previous examples, here the empirical semi-variogram shows no clear asymptotic

behaviour. In other words, variance in brain size was simply proportional to phylogenetic distance. The infinitely diffusive BM model was therefore the most appropriate model for the data, and the semi-variogram shows this correspondence. Thus, even though the OU variogram falls visually closer to the empirical data (Figure 6b), it is not supported because the fit requires an additional parameter.

4 | DISCUSSION

Since Felsenstein (1985) translated the concept of phylogenetic inertia into a statistical problem, methods for modelling evolutionary processes have been advancing rapidly (e.g. Abouheif, 1999; Blomberg et al., 2020; Butler & King, 2004; Harmon et al., 2008; Martins & Hansen, 1997; Revell et al., 2008), allowing for substantially more profound insight into evolutionary biology than was previously possible. While these modelling approaches all treat phylogenetic inertia as a form of statistical autocorrelation, few tools exist to visualise the autocorrelation structure of the trait data and diagnose the fits of evolutionary models (but see the phylogenetic correlograms of Gittleman & Kot, 1990 and Diniz-Filho, 2001 and diversity through time plots of Harvey et al., 1994). As such, researchers often rely on colouring the branch tips or lengths of phylogenetic trees based on trait values (e.g. Revell, 2013). While these can serve as a useful visual tool, they provide only limited on the underlying stochastic process by which the trait may be evolving, and on whether any of the candidate models actually look like the data. For example, a monotonic decrease in diversity over time might indicate a BM process on speciation. Here we extended semi-variograms developed for visualising temporal autocorrelation in other contexts (Fleming et al., 2014) to the needs of phylogenetic autocorrelation, and show how phylogenetic variograms can be used to straightforwardly visualise phylogenetic autocorrelation structures. Notably, because the variograms of the IID, BM and OU processes each have different theoretical profiles, comparing fitted semi-variance functions against empirical semi-variograms can serve as a useful diagnostic tool, allowing researchers to understand why any given evolutionary model might be selected over another, which features are well captured by the model, and which are not.

When modelling musteloid SSD, the empirical variogram showed a tendency for the variance in SSD to stabilise over time, a characteristic feature of OU evolution. In agreement with this visual assessment, AIC-based model selection identified the OU model as the best fit to the data. In contrast, the BM model received substantially less support than the OU model. While AIC-based model selection yielded a clear 'top' model, without the empirical variogram it would not have been possible to see that the failure of the infinitely diffusive BM model was because it did not capture the asymptotic behaviour of the data. Indeed, for musteloid SSD a white noise, IID process was actually a better fit to the variogram than the BM model. The phylogenetic variogram proved equally useful in understanding why the OU model was selected when modelling population growth rate in the Carnivora, and why BM was the selected

evolutionary model for brain size in the Artiodactyla. For the time-scale over which species in the Artiodactyla have been diverging, the variance in brain size has yet to show any evidence of stabilising selection (Figure 6b). Here BM showed good correspondence with the empirical variogram.

It is important to note that while variograms can serve as valuable diagnostic tools, they are only as useful as the pool of models against which they can be compared. In other words, it is entirely possible that none of the candidate models end up being a good match to the data. While variograms on their own do nothing to solve this problem, they do allow research to identify potential pitfalls and areas for model improvement. For instance, the empirical variograms for both growth rate in the Carnivora, and brain size in the Artiodactyla showed strong phylogenetic inertia over shorter time-scales that was not well captured by any of the models fitted here (Figures 5b and 6b). A model with multiple autocorrelation time-scales would likely be a better match to those data (e.g. Fleming et al., 2014; Johnson et al., 2008), and is a promising area of future research. In this regard, however, it is also important to note that variogram errors are correlated (Diggle et al., 1998), and smooth trends may not necessarily be significant and should be treated with caution. Finally, another important limitation of phylogenetic variograms is that the time-lags for phylogenetic variograms are calculated based on the topologies and branch lengths of the supplied phylogenetic trees. As such, the structure of a particular tree will dictate what pairwise time-lags are possible and the resulting time series will almost always be heavily irregular. When combined with pronounced interspecific variability and small sample sizes, phylogenetic variograms can be difficult to interpret. In addition, although we did not assess the impact of tree topology on parameter estimation here, the model fitting process can be strongly affected by the data density across the time-lags. Despite these limitations, however, phylogenetic variograms can serve as a useful tool for visualising the autocorrelation structure of evolutionary processes, and informing future model developments.

When working with autocorrelated data, it is generally recommended that any analysis begin with a nonparametric estimate of the autocorrelation structure of the data that can be visualised. Although this is a key step in the data analysis 'pipeline', it is one that has heretofore not been possible for phylogenetic data (but see Diniz-Filho, 2001; Gittleman & Kot, 1990). The variograms methods developed here enable evolutionary ecologists to visualise phylogenetic autocorrelation from trait data and phylograms or chronograms prior to any model fitting procedure. The theoretical semi-variance functions further allow for fitted models to be compared against the empirical variogram, facilitating model identification, in tandem with standard model selection techniques, prior to subsequent analyses. We therefore recommend that any phylogenetic analysis include variogram estimation and visualisation (see also Pérez-Barbería et al., 2004). The methods developed in this work are openly accessible in the R package `ctpm`, available on CRAN.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

AUTHORS' CONTRIBUTIONS

M.J.N., W.F.F. and C.H.F. contributed to the original project conception and development; M.J.N. developed the `ctpm` R package, analysed the data and drafted the manuscript; C.H.F. derived the weights and aided with the development of the `ctpm` package. All authors contributed to the writing.

PEER REVIEW

The peer review history for this article is available at <https://publons.com/publon/10.1111/2041-210X.13763>.

DATA AVAILABILITY STATEMENT

All data used in the manuscript are currently openly accessible. The musteloid trait data were obtained from Noonan et al. (2015) and the phylogenetic tree from Law et al. (2017). The data on maximum per capita rate of population growth, r , in the Carnivora were obtained from Fagan et al. (2013) and the phylogenetic tree of the Carnivora from Agnarsson et al. (2010). The data on log-scaled mean brain size and the phylogenetic tree of the Artiodactyla are openly available in the R package `slouch` (Toljagić et al., 2018). The `ctpm` R package is available on CRAN and the code necessary to reproduce the analyses in the main text are included as Supporting Information.

ORCID

Michael J. Noonan  <https://orcid.org/0000-0003-4512-0535>

Christen H. Fleming  <https://orcid.org/0000-0002-9356-6518>

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